

1,2-Cyclohexanedicarboxylic acid, ethyl methyl ester

Inchi:	InChI=1S/C11H18O4/c1-3-15-11(13)9-7-5-4-6-8(9)10(12)14-2/h8-9H,3-7H2,1-2H3
InchiKey:	KTQLZENVPSGMMQ-UHFFFAOYSA-N
Formula:	C11H18O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	-409.36	kJ/mol	Joback Method
hf	-725.99	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	58.51	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.529		Crippen Method
mvol	169.870	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1483.00		NIST Webbook
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tb	618.54	K	Joback Method
tc	826.40	K	Joback Method
tf	361.19	K	Joback Method
vc	0.631	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.32	J/molxK	618.54	Joback Method
cpg	474.52	J/molxK	653.18	Joback Method
cpg	490.77	J/molxK	687.83	Joback Method
cpg	506.08	J/molxK	722.47	Joback Method
cpg	520.42	J/molxK	757.11	Joback Method
cpg	533.81	J/molxK	791.76	Joback Method
cpg	546.22	J/molxK	826.40	Joback Method
dvisc	0.0020110	Paxs	361.19	Joback Method

dvisc	0.0011307	Paxs	404.08	Joback Method
dvisc	0.0007100	Paxs	446.97	Joback Method
dvisc	0.0004837	Paxs	489.87	Joback Method
dvisc	0.0003505	Paxs	532.76	Joback Method
dvisc	0.0002665	Paxs	575.65	Joback Method
dvisc	0.0002105	Paxs	618.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339649&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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